

Supplementary Materials

Label-Free Detection of DNA via Surface-Enhanced Raman Spectroscopy Using Au@Ag Nanoparticles

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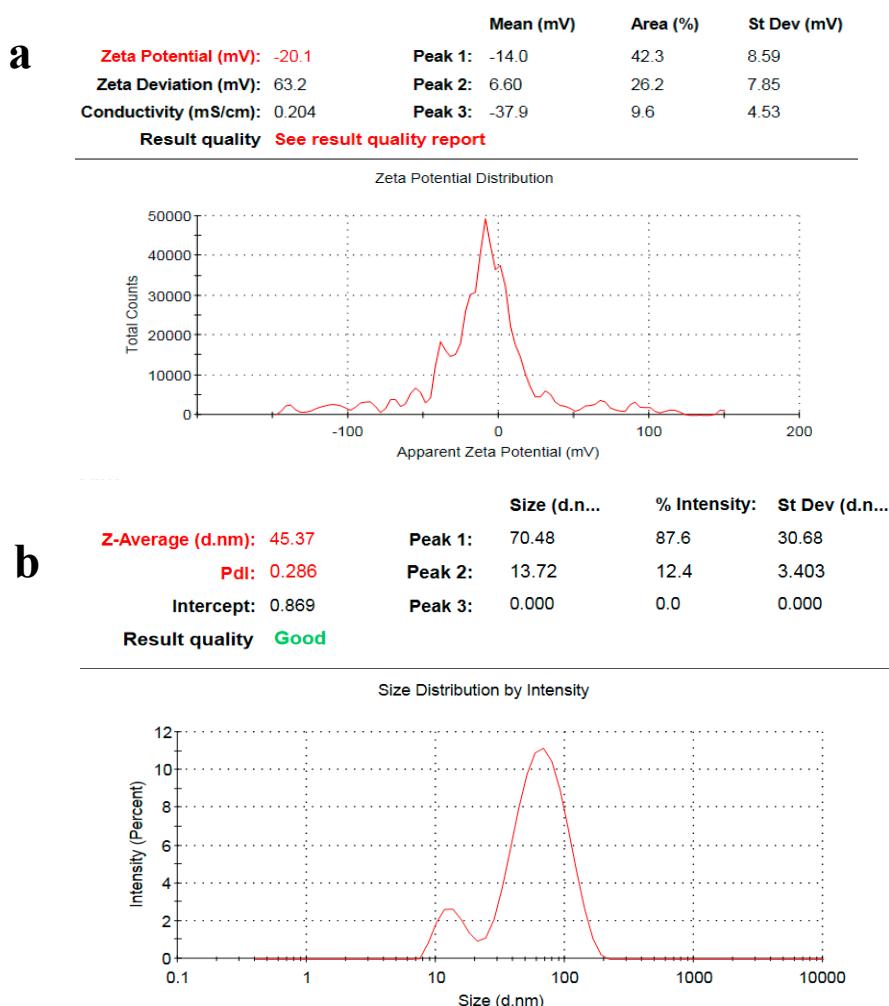


Figure S1. (a)The Zeta potential of Au@AgNPs; (b) The DLS data of Au@AgNPs.

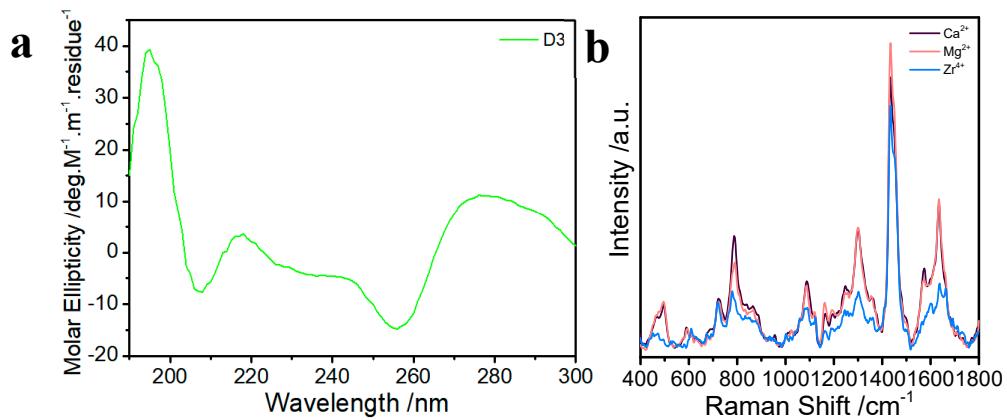


Figure S2. (a) CD spectra of the D3; (b) The D3 SERS spectrum of Au@AgICNPs (Brown line), Au@AgIMNPs (red line) and Au@AgIZNPs (blue line).

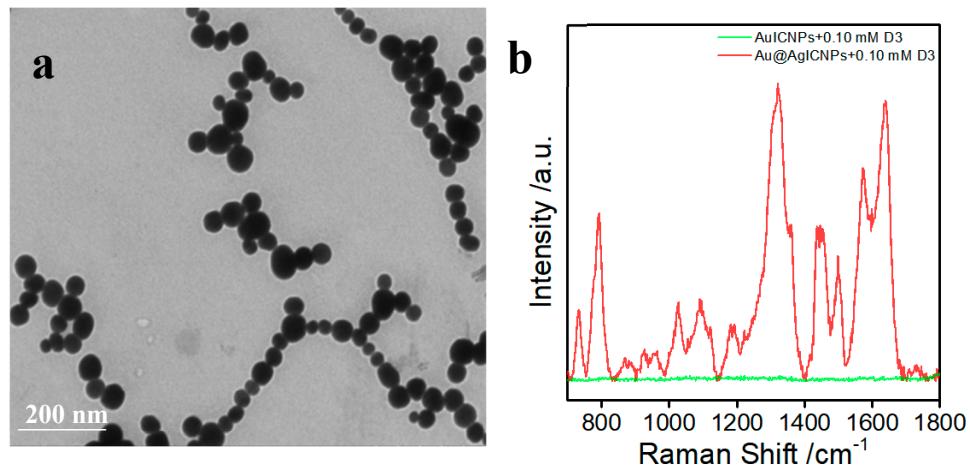


Figure S3. (a) The TEM of pure AuNPs; (b) The D3 SERS spectrum of AuICNPs with 0.1 mM D3 (green line) and Au@AgICNPs with 0.1 mM D3(red line).

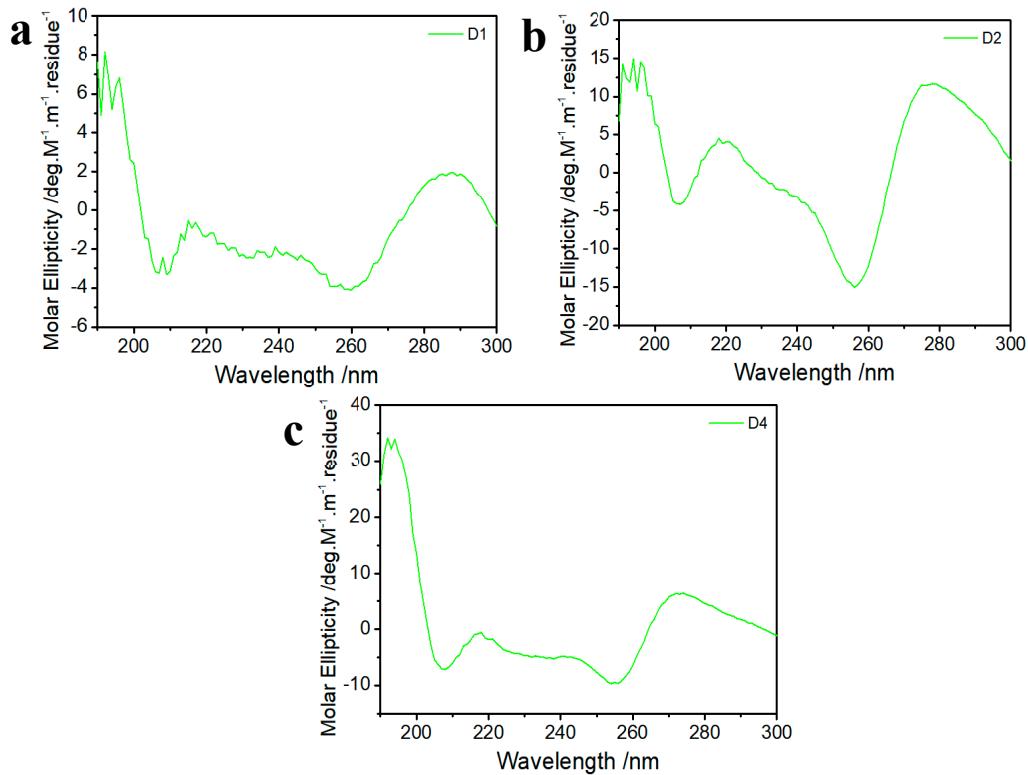


Figure S4. (a) The CD spectra of the D1; (b) The CD spectra of the D2; (c) The CD spectra of the D4.

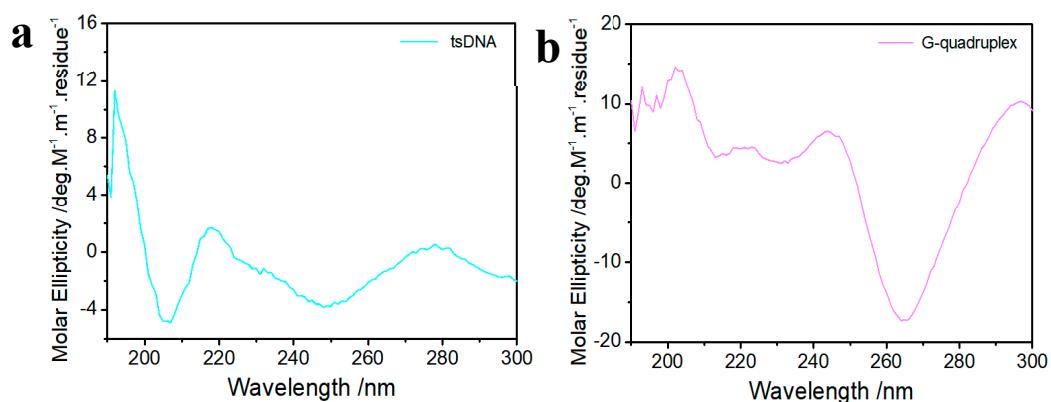


Figure S5. (a) The CD spectra of the tsDNA; (b) The CD spectra of the G-quadruplex.

Table S1. The characteristic peak positions of DNA of different structures.

| Raman Shift | | dsDNA | tsDNA |
|-----------------------|-----------------------|--------------------------------------|--------------------------------------|
| 733 cm ⁻¹ | 736 cm ⁻¹ | dA ring br | dA ring br |
| 789 cm ⁻¹ | 795 cm ⁻¹ | vs OPO; dC ring br | vs OPO; dT ring br |
| 868 cm ⁻¹ | - | v OPO, bk | - |
| 962 cm ⁻¹ | - | d, dG δ R5 | - |
| 1028 cm ⁻¹ | 1033 cm ⁻¹ | d (v C-O) | d (v C-O) |
| 1093 cm ⁻¹ | 1094 cm ⁻¹ | vs PO ₂ ⁻ , bk | vs PO ₂ ⁻ , bk |
| 1323 cm ⁻¹ | 1322 cm ⁻¹ | dG v(C-N) δ(C8-H) | dG v(C-N) δ(C8-H) |
| 1360 cm ⁻¹ | - | dG C2'-endo/ <i>syn</i> | - |
| 1637 cm ⁻¹ | 1632 cm ⁻¹ | dT, dC v C5=C6 | dT v C5=C6 |

| Raman Shift | | dsDNA | G-quadruplex |
|-----------------------|-----------------------|--------------------------------------|---|
| 733 cm ⁻¹ | 713 cm ⁻¹ | dA ring br | dA ring br |
| 789 cm ⁻¹ | 789 cm ⁻¹ | vs OPO; dC ring br | vs OPO; dT ring br |
| 868 cm ⁻¹ | - | v OPO, bk | - |
| 962 cm ⁻¹ | - | d, dG δ R5 | - |
| 1028 cm ⁻¹ | - | d (v C-O) | - |
| 1093 cm ⁻¹ | 1087 cm ⁻¹ | vs PO ₂ ⁻ , bk | vs PO ₂ ⁻ , bk |
| - | 1241 cm ⁻¹ | - | dT, dG δ NH(N2) |
| 1323 cm ⁻¹ | - | dG v(C-N) δ(C8-H) | - |
| 1360 cm ⁻¹ | 1358 cm ⁻¹ | dG C2'-endo/ <i>syn</i> | dG v(C-N) δ(C8-H) C2'- endo/ <i>anti</i> |
| 1637 cm ⁻¹ | 1644 cm ⁻¹ | dT, dC v C5=C6 | dT v C5=C6 |
| - | 1764 cm ⁻¹ | - | dG v C=O (O6 interbase H- bond) |

Note: bk=DNA - phosphate backbone, d =deoxyribose, v=stretch, δ=deformation, br =breathe, s =symmetry.

Table S2. The motifs of tsDNA and G-quadruplex detected in the paper.

| tsDNA | 5'-AGA γ GGA-3' 5'-TCT γ CCT-3' |
|--------------|---|
| G-quadruplex | 5'-G ₄ T ₄ G ₄ -3' |